

Acetone, O-isopropylloxime

Inchi:	InChI=1S/C6H13NO/c1-5(2)7-8-6(3)4/h6H,1-4H3
InchiKey:	LHEAKOCZFQCLGM-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CC(C)=NOC(C)C
Mol. weight [g/mol]:	115.17

Physical Properties

Property code	Value	Unit	Source
hf	-232.24	kJ/mol	Joback Method
hvap	34.37	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.807		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	724.00		NIST Webbook
tb	435.22	K	Joback Method
tc	630.49	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logP:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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<https://www.chemeo.com/cid/35-674-5/Acetone-O-isopropylloxime.pdf>

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